PB86-213246

Study Using a Three-Dimensional Smog Formation Model under Conditions of Complex Flow

(U.S.) National Research Council, Washington, DC

Prepared for

Environmental Protection Agency
Research Triangle Park, NC

May 86

U.S. Department of Commerce
National Technical Information Service
NTIS

PB86-213246

EPA/600/D-86/116
May 1986

A STUDY USING A THREE-DIMENSIONAL SMOG FORMATION MODEL UNDER CONDITIONS OF COMPLEX FLOW

by

S. Wakamatsu*, K. L. Schere**, J. H. Shreffler**, and I. Uno*

EPA Project Officer
K. L. Schere

EPA Grant CR812483

* National Institute for Environmental Studies, Tsukuba, Ibaraki 305, Japan
**Atmospheric Sciences Research Laboratory, U.S. EPA, Research Triangle Park, NC 27711

ATMOSPHERIC SCIENCES RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA
(Please read instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
EPA/600/D-86/116		PB86-213246/AS

4. TITLE AND SUBTITLE	5. REPORT DATE
A STUDY USING A THREE-DIMENSIONAL PHOTOCHEMICAL SMOG FORMATION MODEL UNDER CONDITIONS OF COMPLEX FLOW	May 1986
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)	8. PERFORMING ORGANIZATION REPORT NO.
S. Wakamatsu, K.L. Schere, J.H. Shreffler, and I. Uno	
9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT NO.
National Research Council 2101 Constitution Ave. Washington, D.C. 20418	CDWA1A/04-4175 (FY-86)
	11. CONTRACT/GRANT NO.
	CR812483-01
12. SPONSORING AGENCY NAME AND ADDRESS	13. TYPE OF REPORT AND PERIOD COVERED
Atmospheric Sciences Research Laboratory - RTP, NC Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, North Carolina 27711	14. SPONSORING AGENCY CODE EPA/600/09

15. SUPPLEMENTARY NOTES

16. ABSTRACT

To clarify the photochemical smog formation mechanisms under conditions of complex flow, the SAI Urban Airshed Model was evaluated using a 1981 field observed data base. In the Tokyo Metropolitan Area higher O_3 concentrations are usually observed near the shore in the morning. As the sea breeze layer penetrates inland, this high concentration region travels with it, increasing in concentration with time. A nighttime radiation inversion which persists into the early morning prevents the dispersion of primary pollutants emitted from the big coastal industrial zones and the Tokyo Metropolitan Area. Usually, aged high O_3 concentrations are observed aloft in the early morning, and these are entrained into the mixing layer in accordance with the elevation of the lid. This effect is believed to accelerate the formation of secondary pollutants during the next day. The quantitative role and weight of the previous day's secondary pollutants, newly emitted pollutants, temporal variation of mixing height and three-dimensional wind field for the O_3 formation mechanisms were investigated. The three-dimensional simulated results showed good quantitative agreement with the observed field data but underestimated the aircraft data.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS (This Report)	21. NO. OF PAGES
RELEASE TO PUBLIC	UNCLASSIFIED	11
	20. SECURITY CLASS (This page)	22. PRICE
	UNCLASSIFIED	$9.95

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

NOTICE

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

A STUDY USING A THREE-DIMENSIONAL SMOG FORMATION MODEL UNDER CONDITIONS OF COMPLEX FLOW

S. WAKAMATSU*, K.L. SCHERE**, J.H. SHREFFLER**, and I. UNO*

* National Institute for Environmental Studies,
P.O. Yatabe, Tsukuba, Ibaraki 305, JAPAN
** Atmospheric Sciences Research Laboratory,
U.S. EPA, Research Triangle Park, N.C. 27711, U.S.A.

SUMMARY

To clarify the photochemical smog formation mechanisms under conditions of complex flow, the SAI Urban Airshed Model was evaluated using observations from a 1981 field experiment. In the Tokyo Metropolitan Area higher O_3 concentrations are usually observed near the shore in the morning. As the sea breeze layer penetrates inland, this high concentration region travels with it, increasing in concentration with time. A nighttime radiation inversion which persists into the early morning prevents the dispersion of primary pollutants emitted from the big coastal industrial zones and the Tokyo Metropolitan Area. Usually, aged high O_3 concentrations are observed aloft in the early morning, and these are entrained into the mixed layer in accordance with the elevation of the lid. This effect is believed to accelerate the formation of secondary pollutants during the next day. The quantitative role and weight of the previous day's secondary pollutants, temporal variation of mixing height and three-dimensional wind field for the O_3 formation mechanisms were investigated. The three-dimensional simulated results showed good agreement with the observed field data but underestimated the aircraft data.

INTRODUCTION

During July 16 and 17, 1981 high O_3 concentrations were observed in the Tokyo Metropolitan Area under the condition of a complex wind field. During this period, intensive field measurements of vertical and horizontal wind and pollutants were made. The weather conditions were typical of this season in Japan. A predominant northern Pacific high pressure cell with weak gradients covered the Japanese archipelago. Under these conditions, especially high oxidant concentrations were observed in the southern part of the Tokyo Metropolitan Area due to the orientation of the sea-land breeze circulation system to the metropolitan area. To further understand these phenomena, the SAI Urban Airshed Model (UAM) was applied.

SIMULATION METHODS

The UAM is a three-dimensional Eulerian, photochemical air quality simulation model developed by Systems Applications, Inc. of San Rafael, California, U.S.A.[1] The area modeled around Tokyo was 183 km wide and

172 km long with each individual cell 6.8 km wide and 5.5 km long. Vertically, there were five layers of cells in total; the bottom three layers simulated the mixed layer and the top two represented the region above the mixed layer. However, when the mixing layer exceeded 1000 m, the five layers were fixed at constant altitudes. The top height of the region was 2000 m. Figures 1 and 2 show a horizontal and vertical cross-section of the domain, respectively. The model simulation was conducted for 40 hours beginning 0400 JST, July 16, 1981. Data from 62 selected ground monitoring stations, 4 upper-air sounding sites, and 23 pilot balloon sites were used to determine the boundary concentrations and the meteorological parameter values for the model input. The aircraft measurements showed a very complex vertical and horizontal pollutant distribution, mainly caused by the complex wind structure. To simulate this wind field, a three-dimensional mass and momentum-conserving wind model was used.(2) The Carbon Bond chemical kinetic scheme was used for chemistry calculations. Hourly emission rates were calculated from area sources and point sources for NO_x and non-methane hydrocarbons at each grid cell. Non-methane hydrocarbon (NMHC) emissions must be distributed into particular structure classes. To do this the ratio of 18 NMHC species from the five major hydrocarbon sources were determined.(3)

RESULTS AND DISCUSSION

Calculated diurnal variations of O_3 for 12 selected monitoring stations are shown in Figure 4 with the observed O_3 concentrations. The locations of these stations are mapped in Figure 3. In the daytime the calculated values show good agreement with the observed data; however at night observed oxidant concentrations decrease more rapidly than the simulated O_3. Near the monitoring station in Yokohama there are large NO_x elevated point emission sources and for this reason the ground-level oxidant concentration is overestimated. This is mainly caused by the quenching effects on O_3. Figure 5(a) shows observed oxidants and the surface wind distribution at 1600 JST on July 16, 1981. The simulated aerial distribution in Figure 5(b) shows good agreement with observations. Primary pollutants emitted from the large industrial complexes around Tokyo Bay and the Tokyo metrolpolis were trapped in the sea breeze region from Sagami Bay and produced high O_3 in the southern part of the Kanto Plain.

Aircraft measurements were conducted 6 times per day. In each of the 12 runs, sample air was collected in a glass vessel and hydrocarbon species were analyzed after the flight. NO_x and O_3 measurements were made continuously. Table 1(a) shows averaged values of hydrocarbon, NO_x, and O_3 concentrations. The values listed are the averaged values while air was being sampled for hydrocarbon analysis. Average flight altitude was approximately between 350 m and 650 m. Table 1(b) shows an example of the simulation in Yokohama at 1600 and 2400 JST, July 16, and 0600 JST, July 17, 1981. Aircraft observations at 1600 JST correspond to the simulation of model Layer 2, and the observations of 0600 JST correspond to Layer 3. Comparing Tables 1(a) and 1(b), PAR and ARO measured by the aircraft were higher than the simulated values. CARB was not measured in the aircraft study. This discrepancy might be caused from the estimation error of hydrocarbon emission intensity. Calculated vertical distributions in Table

1(b) showed good qualitative agreement with the aircraft data. In the nighttime and early morning, higher NO_x concentrations were observed in the lower layer and higher O_3 in the upper layer. In the daytime, pollutants diluted too rapidly and showed uniform distributions in the mixing layer. Usually the aircraft-observed data showed a peak in O_3 concentration in Layer 3. Figure 6 shows the comparison between the diurnal variation of O_3 measured by aircraft and the simulation. Simulated values were obtained by averaging the calculated mesh values located inside of the flight course. A typical flight path is shown in Figure 3. Simulated values underestimated th aircraft data.

CONCLUSIONS

To investigate the photochemical smog formation mechanisms under conditions of complex flow in the Tokyo Metropolitan Area, the SAI Urban Airshed Model was evaluated. It was found that:

(1) The SAI Urban Airshed Model produced reasonable calculated results for the diurnal and aerial distributions of O_3 concentration covering the Tokyo Metropolitan Area.
(2) The diurnal variation of vertical distributions of NO_x, hydrocarbons, and O_3 showed good agreement with the aircraft data, but during the daytime, pollutants were well distributed vertically and showed a uniform profile.
(3) Usually the aircraft data showed sharp O_3 peaks near the top of the mixing layer during the daytime[4],[5]; the model did not show these peaks. This discrepancy may be caused by the incorrect treatment of vertical mixing in the model.
(4) PAR and ARO concentrations were underestimated. This might be caused from the estimation error in the hydrocarbon emissions.

REFERENCES

(1) Ames,J., Myers,T.C., Reid,L.E., Whitney,D.C., Golding,S.H., Hayes,S.R., and Reynolds,S.D. 1985: SAI Airshed Model operations manuals. Vol. 1 - User's manual. EPA-600/8-85/007a, U.S. Environmental Protection Agency, Research Triangle Park, N.C., U.S.A.
(2) Fosberg,M.A. 1984: A diagnostic three-dimensional mass and momentum conserving wind model for complex terrain. Third conference on mountain meteorology. American Meteorological Society, Boston, MA, U.S.A.
(3) Wakamatsu,S., Uno,I., and Wadden,R.A. 1984: A study of NMHC source fingerprint and its photochemical reactivity. 8th U.S.-Japan Conference on Photochemical Pollution.
(4) Wakamatsu,S., Ogawa,Y., Murano,K., Goi,K., and Aburamoto,Y. 1983: Aircraft survey of the secondary photochemical pollutants covering the Tokyo Metropolitan Area. Atmos. Environ., 17, 827-835.
(5) Uno,I., Wakamatsu,S., Suzuki,M., and Ogawa,Y. 1984: Three-dimensional behavior of photochemical pollutants covering the Tokyo Metropolitan Area. Atmos. Environ., 18, 751-761.

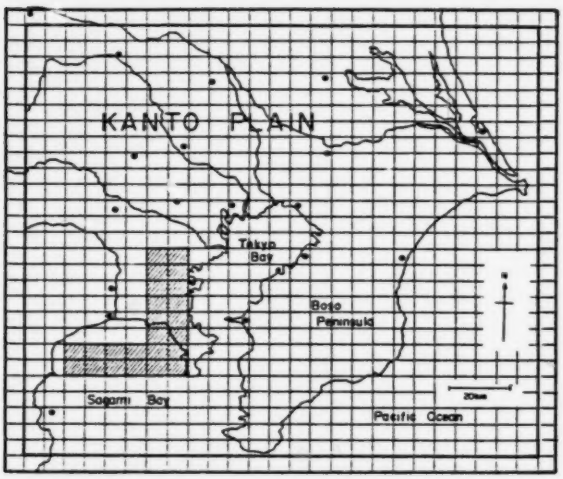

Fig.1 Schematic drawing of horizontal section of UAM domain.

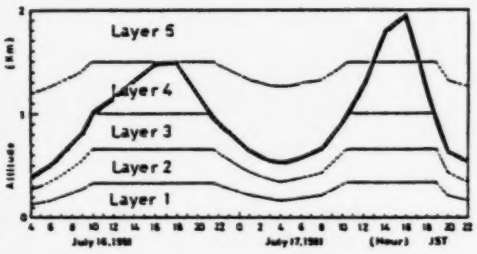

Fig.2

Schematic drawing of vertical Layer structure of UAM.

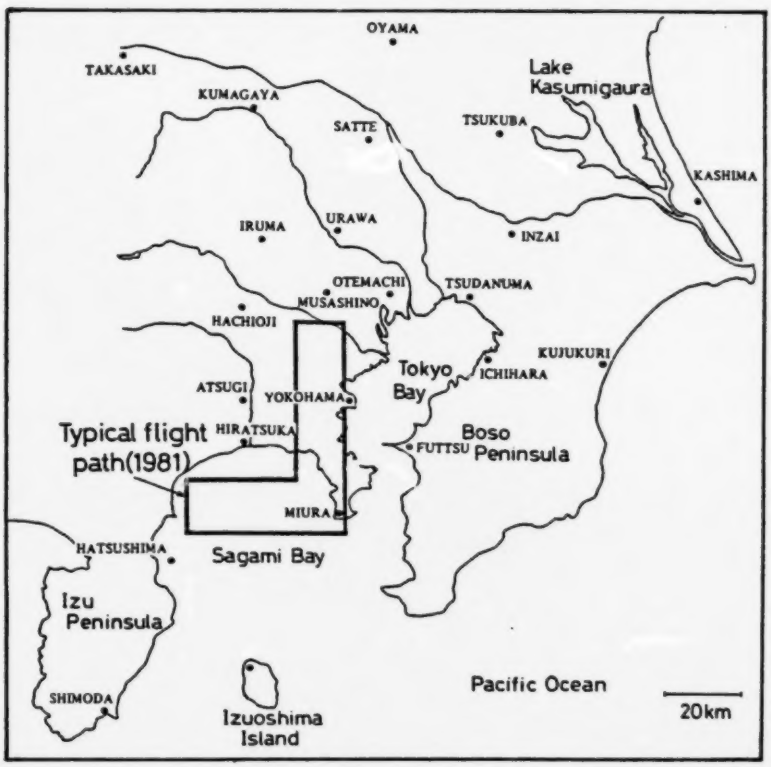

Fig.3 Topography of Tokyo Metropolitan Area and typical flight path. Dot shows pilot-balloon observation points.

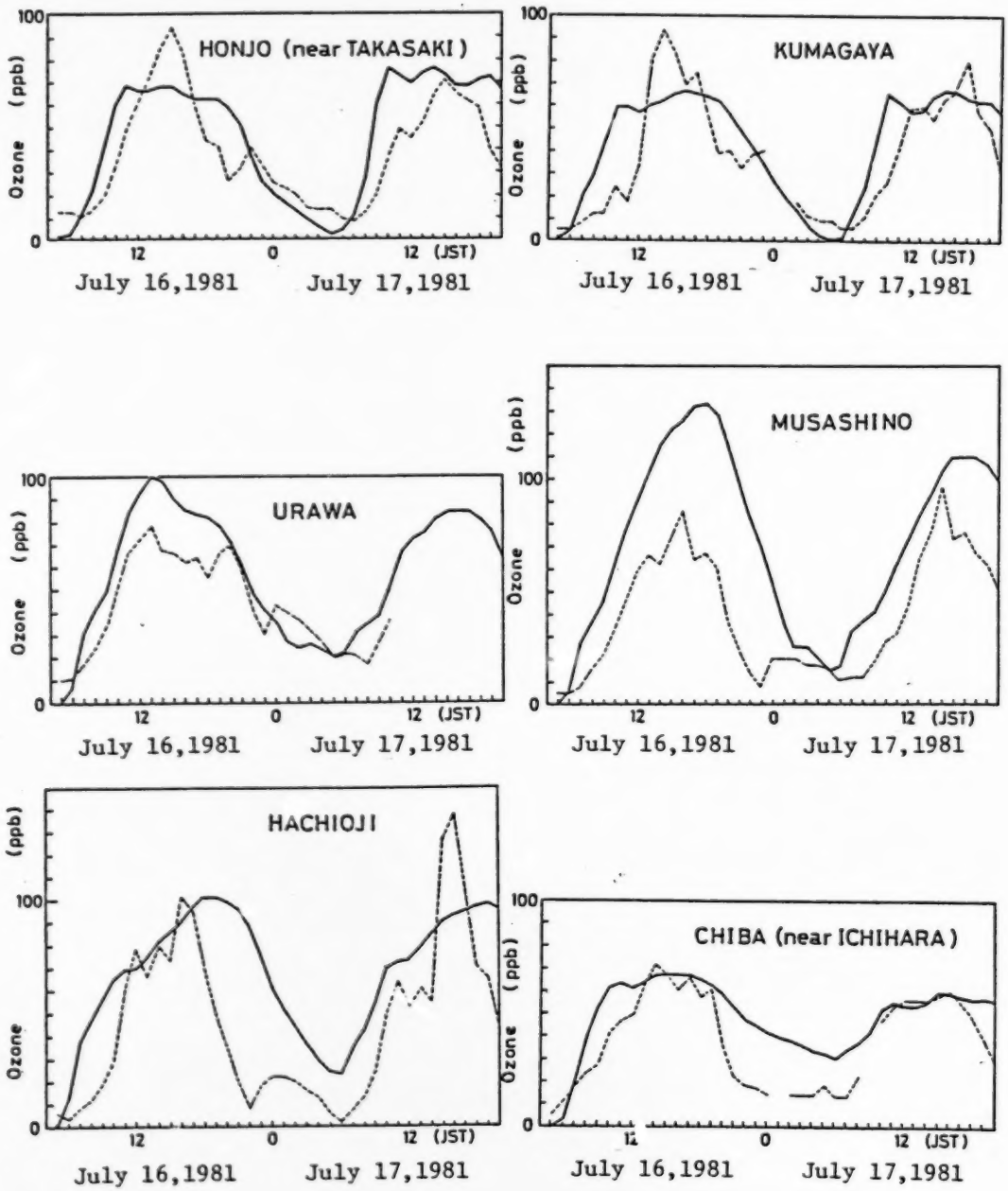

Fig.4(a) Diurnal variation of O_3 on July 16 17,1981. Solid line shows the simulated hourly averaged O_3 values for Layer 1 of UAM and dashed line shows ground level monitoring O_3 data. The location of each monitoring station is shown in Figure 3.

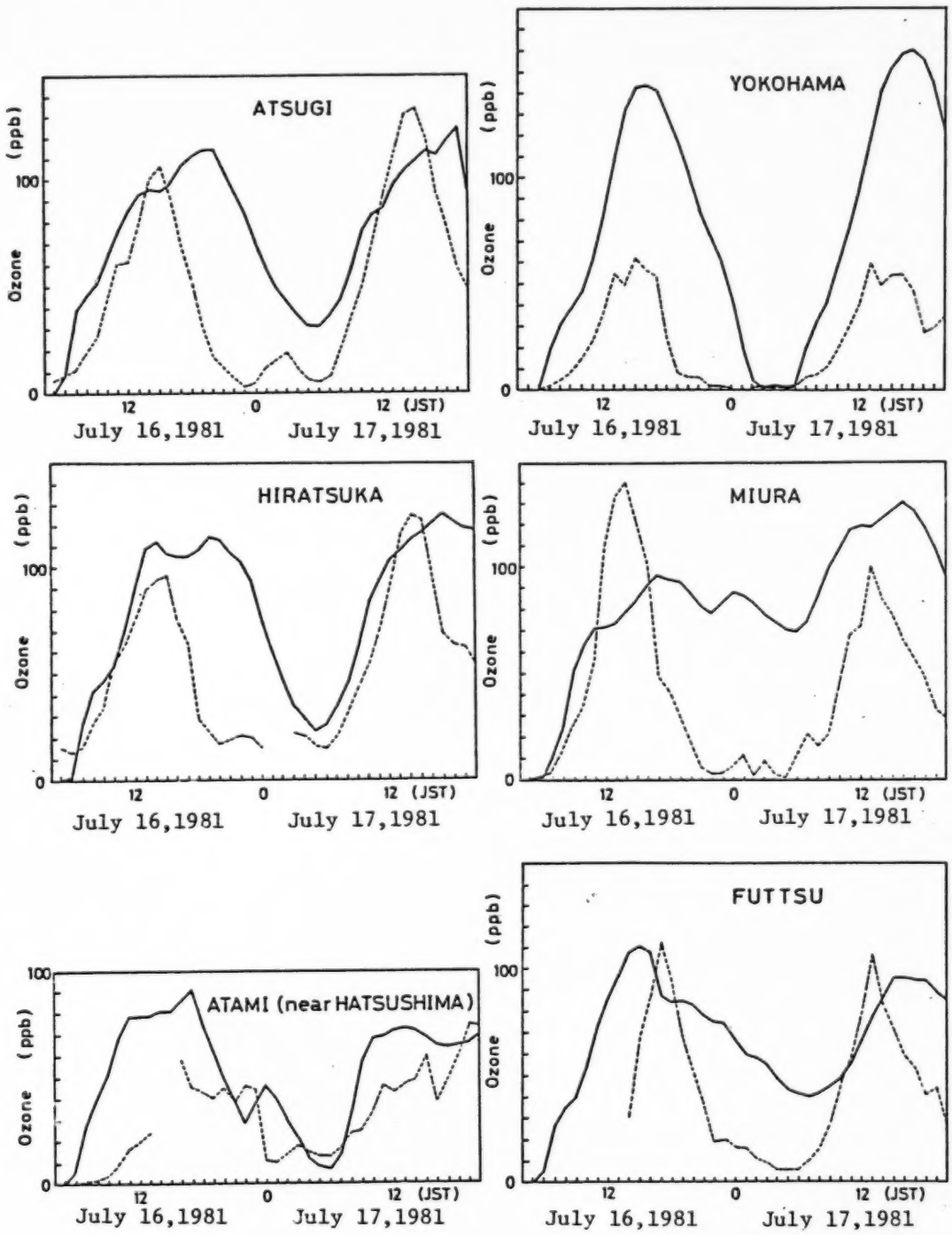

Fig.4(b) Diurnal variation of O_3 on July 16 17,1981. Solid line shows the simulated hourly averaged O_3 values for Layer 1 of UAM and dashed line shows ground level monitoring O_3 data. The location of each monitoring station is shown in Figure 3.

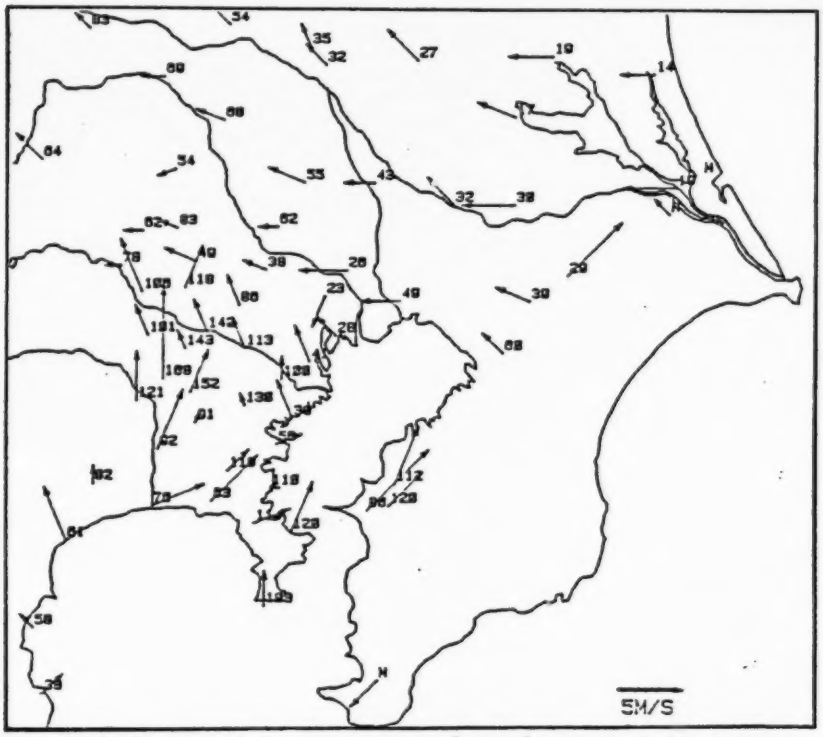

Fig.5(a) Observed O_3 pattern and surface wind distribution at 1600JST on July 16,1981.

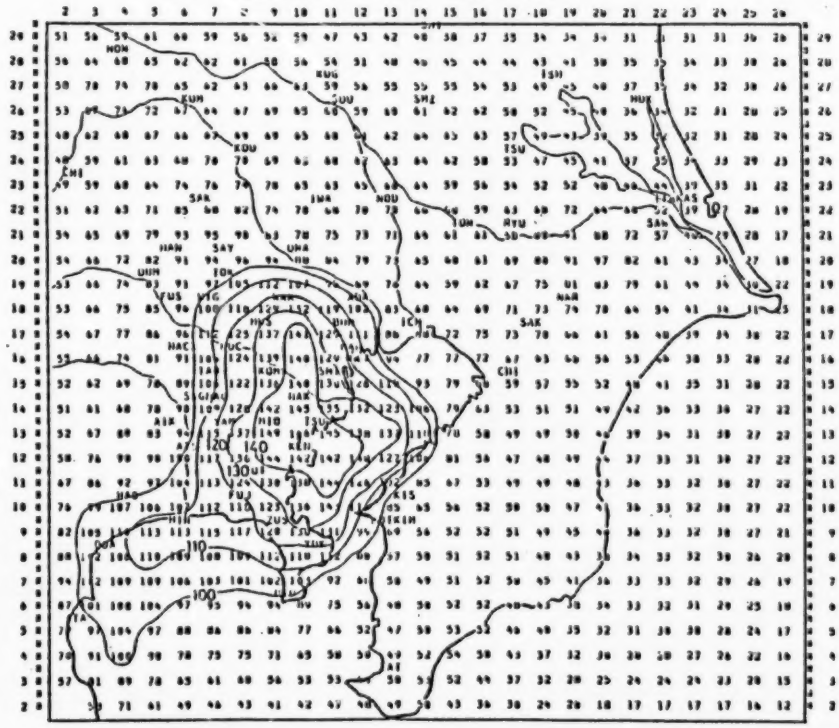

Fig.5(b) Simulated hourly-averaged O_3 concentration in Layer 1 at 1500-1600JST on July 16,1981.

Aircraft data (Observed data)

RUN	DAY (1981)	HOUR (JST)	N	Pollutants (ppb) NO	NO_2	O_3	ETH	OLE	PAR	ARO
11		0529-0716	23	6	9	36	4	1	92	24
12		0852-1037	18	7	11	85	7	1	139	23
13		1155-1308	19	5	14	164	5	1	227	26
14	July 16	1435-1543	11	7	12	173	5	0	197	21
15		1721-1831	11	4	10	158	3	0	161	22
16		2010-2127	12	4	14	124	2	0	138	18
21		0520-0653	24	5	16	51	9	2	185	24
22		0824-0955	20	5	15	89	7	1	163	23
23		1131-1241	20	0	21	171	5	0	253	29
24	July 17	1420-1531	12	5	18	188	3	0	191	21
25		1718-1818	12	0	11	169	2	0	130	19
26		2008-2107	11	4	8	129	3	0	134	20

Table 1(a) Average concentration of aircraft observation for each RUN.

YOKOHAMA (Simulated results)

Pollutants (ppb)	Day (1981)	Hour (JST)	Layer1	Layer2	Layer3	Layer4	Layer5
NO	July 16,	1600	1	1	1	1	0
	16,	2400	0	0	0	0	0
	17,	0600	4	1	0	0	0
NO2	July 16,	1600	7	6	5	5	4
	16,	2400	45	34	19	6	4
	17,	0600	56	54	42	6	3
O3	July 16,	1600	144	144	143	142	138
	16,	2400	43	83	94	68	61
	17,	0600	2	20	34	41	47
ETH	July 16,	1600	3	3	2	2	2
	16,	2400	6	4	3	1	1
	17,	0600	18	11	5	2	1
OLE	July 16,	1600	0	0	0	0	0
	16,	2400	1	1	0	0	0
	17,	0600	3	2	1	0	0
PAR	July 16,	1600	91	87	86	84	80
	16,	2400	109	84	68	38	32
	17,	0600	193	132	78	46	28
CARB	July 16,	1600	26	25	25	24	23
	16,	2400	20	22	20	11	8
	17,	0600	24	21	15	5	5
ARO	July 16,	1600	4	4	3	3	3
	16,	2400	12	8	6	3	2
	17,	0600	32	19	10	8	3

Table 1(b) Simulated results in Yokohama at 1600,2400JST July 16,1981 and 0600JST July 17,1981.

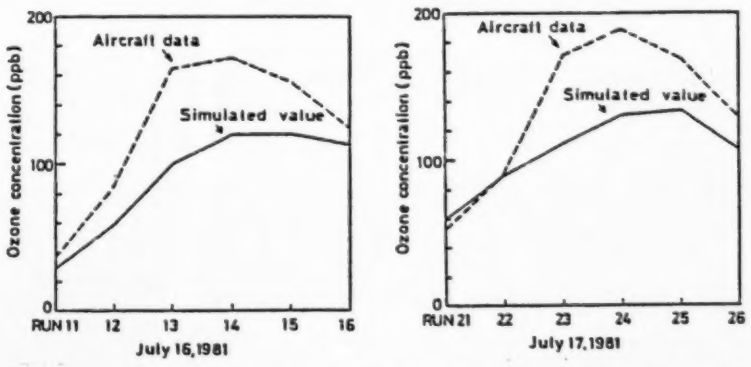

Fig.6 Comparison between aircraft data and simulated values on July 16,1981 and on July 17,1981. Simulated value is the averaged value within the area encompassed by each flight path.